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Strange effect of disorder on electron transport through a thin film

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Abstract

A novel feature of electron transport is explored through a thin film of varying impurity density with the distance from its surface. The film, attached to two metallic electrodes, is described by simple tight-binding model and its coupling to the electrodes is treated through Newns-Anderson chemisorption theory. Quite interestingly it is observed that, in the strong disorder regime the amplitude of the current passing through the film increases with the increase of the disorder strength, while it decreases in the weak disorder regime. This anomalous behavior is completely opposite to that of conventional disordered systems. Our results also predict that the electron transport is significantly influenced by the finite size of the thin film.

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1 Introduction

In the last few decades considerable attention has been paid to the propagation of electrons through quantum devices with various geometric structures where the electron transport is predominantly coherent [1, 2]. Recent progress in creating such quantum devices has enabled us to study the electron transport through them in a very tunable environment. By using single molecule or cluster of molecules it can be made possible to construct the efficient quantum devices that provide a signature in the design of future nano-electronic circuits. Based on the pioneering work of Aviram and Ratner [3] in which a molecular electronic device has been predicted for the first time, the development of a theoretical description of molecular electronic devices has been pursued. Later, several experiments [4, 5, 6, 7, 8] have been performed through different molecular bridge systems to understand the basic mechanisms underlying such transport. Though electron transport properties through several bridge systems have been described elaborately in lot of theoretical as well as experimental papers, but yet the complete knowledge of the conduction mechanism in this scale is not well understood even today. For example, it is not so transparent how the molecular transport is affected by its coupling with the side attached electrodes or by the geometry of the molecule itself. Several significant factors are there which control the the electron conduction across a bridge system and all these effects have to be considered properly to study the electron transport. In a their work, Ernzerhof *et al.* [9] have manifested a general design principle through some model calculations, to show how the molecular structure plays a key role in determining the electron transport. The molecular coupling with the electrodes is also another important factor that controls the current in a bridge system. In addition to these, the quantum interference of electron waves [10, 11, 12, 13, 14, 15, 16, 17, 18] and the other parameters of the Hamiltonian that describe the system provide significant effects in the determination of the current through the bridge system. Now in these small-scale devices, dynamical fluctuations play an active role which can be manifested through the measurement of "shot noise", a direct consequence of the quantization of charge. It can be used to obtain information on a system which is not available directly through the conductance measurements, and is generally more sensitive to the effects of electron-electron correlations than the average conductance [19, 20].

In this present paper, we will describe quite a different aspect of quantum transport than the above mentioned issues. Using the advanced nanoscience and technology, it can be made possible to fabricate a nano-scale device where the charge carriers are scattered mainly from its surface boundaries [21, 22, 23, 24, 25] and not from the inner core region. It is completely opposite to that of a traditional doped system where the dopant atoms are distributed uniformly along the system. For example, in shell-doped nanowires the dopant atoms are spatially confined within a few atomic layers in the shell region of a nanowire. In such a shell-doped nanowire, Zhong and Stocks [22] have shown that the electron dynamics undergoes a localization to quasi-delocalization transition beyond some critical doping. In other very recent work [24], Yang *et al.* have also observed the localization to quasi-delocalization transition in edge disordered graphene nanoribbons upon varying the strength of the edge disorder. From the extensive studies of the electron transport in such systems where the dopant atoms are not distributed uniformly along the system, it has been suggested that the surface states [26], surface scattering [27] and the surface reconstructions [28] may be responsible to exhibit several diverse transport properties. Motivated by such kind of systems, in this article we consider a special type of thin film where disorder strength varies smoothly from layer to layer with the distance from the film surface. This system shows a peculiar behavior of the electron transport where the current amplitude increases with the increase of the disorder strength in the limit of strong disorder, while the amplitude decreases in the weak disorder limit. On the other hand, for the conventional disordered system i.e., the system subjected to uniform disorder, the current amplitude always decreases with the increase of the disorder strength. From our study it is also observed that the electron transport through the film is significantly influenced by its size which reveals the finite quantum size effects. Here we reproduce an analytic approach based on the tight-binding model to investigate the electron transport through the film system, and adopt the Newns-Anderson chemisorption model [29, 30, 31] for the description of the electrodes and for the interaction of the electrodes with the film.

We organize this paper as follows. In Section 2, we describe the model and the methodology for the calculation of the transmission probability (T) and the current (I) through a thin film attached to two metallic electrodes by the use of Green's function technique. Section 3 discusses the significant re-

sults, and finally , we summarize our results in Section 4.

2 Model and the theoretical description

This section describes the model and the methodology for the calculation of the transmission probability (T), conductance (g) and the current (I) through a thin film attached to two one-dimensional metallic electrodes by using the Green's function

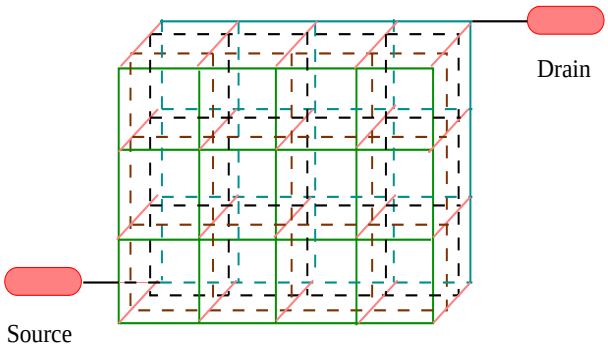

Figure 1: A thin film of four layers attached to two metallic electrodes (source and drain), where the different layers are subjected to different impurity strengths. The top most front layer (green color) is subjected to the highest impurity strength and the strength of the impurity decreases smoothly towards the bottom layer keeping the lowest bottom layer (light blue color) as impurity free. The two electrodes are attached at the two extreme corners of the bottom layer.

technique. The schematic view of such a bridge system is illustrated in Fig. 1.

For low bias voltage and temperature, the conductance g of the film is determined by the Landauer conductance formula [32],

$$g = \frac{2e^2}{h} T \tag{1}$$

where the transmission probability T becomes [32],

$$T = \mathrm{Tr}\left[\Gamma_S G_F^r \Gamma_D G_F^a\right] \tag{2}$$

Here G_F^r and G_F^a correspond to the retarded and advanced Green's functions of the film, and Γ_S and Γ_D describe its coupling with the source and the drain, respectively. The Green's function of the film is written in this form,

$$G_F = \left(E - H_F - \Sigma_S - \Sigma_D\right)^{-1} \tag{3}$$

where E is the energy of the injecting electron and H_F represents the Hamiltonian of the film which can be written in the tight-binding form within the non-interacting picture like,

$$H_F = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{<ij>} t\left(c_i^\dagger c_j + c_j^\dagger c_i\right) \tag{4}$$

In this expression, ϵ_i's are the site energies and t corresponds to the nearest-neighbor hopping strength. As an approximation, we set the hopping strengths along the longitudinal and the transverse directions in each layer of the film are identical with each other which is denoted by the parameter t. Similar hopping strength t is also taken between two consecutive layers, for simplicity. Now in order to introduce the impurities in the thin film where the different layers are subjected to different impurity strengths, we choose the site energies (ϵ_i's) randomly from a "Box" distribution function such that the top most front layer becomes the highest disordered layer with strength W and the strength gradually decreases to-wards the bottom layer as a function of W/N_l (N_l be the total number of layers in the film), keeping the lowest bottom layer as impurity free. On the other hand, in the traditional disordered thin film all the layers are subjected to the same disorder strength W. In our present model we use the similar kind of tight-binding Hamiltonian as prescribed in Eq.(4) to describe the side attached electrodes, where the site energy and the nearest-neighbor hopping strength are represented by the symbols ϵ_i' and v, respectively. The parameters Σ_S and Σ_D in Eq.(3) correspond to the self-energies due to coupling of the film with the source and the drain, respectively, where all the informations of this coupling are included into these two self-energies and are described by the Newns-Anderson chemisorption model [29, 30, 31]. This Newns-Anderson model permits us to describe the conductance in terms of the effective film properties multiplied by the effective state densities involving the coupling, and allows us to study directly the conductance as a function of the properties of the electronic structure of the film between the electrodes.

The current passing through the film can be regarded as a single electron scattering process between the two reservoirs of charge carriers. The current-voltage relationship can be obtained from the expression [32],

$$I(V) = \frac{e}{\pi\hbar} \int_{-\infty}^{\infty} \left(f_S - f_D\right) T(E) dE \tag{5}$$

where $f_{S(D)} = f\left(E - \mu_{S(D)}\right)$ gives the Fermi distribution function with the electrochemical potential $\mu_{S(D)} = E_F \pm eV/2$. Usually, the electric field inside the thin film, especially for small films, seems to have a minimal effect on the g-E characteristics. Thus it introduces very little error if we assume that, the entire voltage is dropped across the film-electrode interfaces. The g-E characteristics are not significantly altered. On the other hand, for larger system sizes and higher bias voltage, the electric field inside the film may play a more significant role depending on the size and the structure of the film [33], but yet the effect is quite small.

In this article, we concentrate our study on the determination of the typical current amplitude which can be expressed through the relation,

$$I_{typ} = \sqrt{< I^2 >_{W,V}} \tag{6}$$

where W and V correspond to the impurity strength and the applied bias voltage, respectively.

Throughout this article we study our results at absolute zero temperature, but the qualitative behavior of all the results are invariant up to some finite temperature ($\sim$ 300 K). The reason for such an assumption is that the broadening of the energy levels of the thin film due to its coupling with the electrodes is much larger than that of the thermal broadening. For simplicity, we take the unit $c = e = h = 1$ in our present calculations.

3 Results and discussion

Here we focus the significant results and describe the strange effect of impurity on electron transport through a thin film subjected to the smoothly varying impurity density from its surface. These results provide the basic conduction mechanisms and the essential principles for the control of electron transport in a bridge system. An anomalous feature of the electron transport through this system is observed, where the current amplitude increases with the increase of the impurity strength in the strong impurity regime, while the current amplitude decreases with the impurity strength in the weak impurity regime. This peculiar behavior is completely opposite to that of the traditional doped film in which the current amplitude always decreases with the increase of the doping concentration. Throughout our discussion we choose the values of the different parameters as follows: the coupling strengths of the film to the electrodes $\tau_S = \tau_D = 1.5$, the hopping strengths $t = 2$ and $v = 4$ respectively in the film and and in the two electrodes. The site energies (ϵ_i''s) in the electrodes are set to zero, for the sake of simplicity. In addition to these parameters, three other parameters are also introduced those are represented by N_x, N_y and N_z, where the first two of them correspond to the total number of lattice sites in each layer of the film along the x and y directions, respectively, and the third one (N_z) represents the total number lattice sites along the z direction of the film. In the smoothly varying disordered film, the different layers are subjected to the strengths $W_l = W/N_l$, keeping the top most front layer as the highest disordered layer with strength W and the lowest bottom layer as disorder free. While, for the conventional disordered film, all the layers are subjected to the identical strength W. Now both for these two cases, we choose the site energies randomly from a "Box" distribution

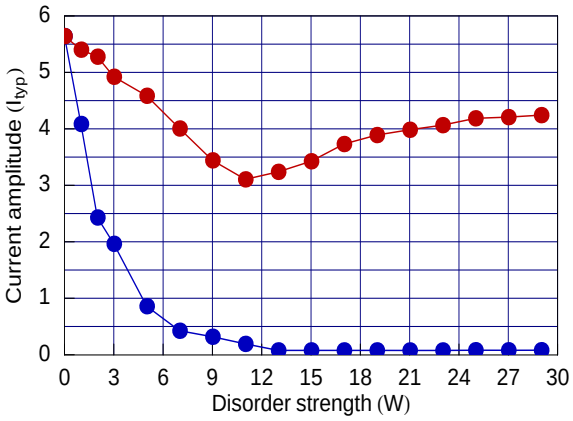

Figure 2: Typical current amplitudes (I_{typ}) as a function of the impurity strength (W) for the thin films with six layers ($N_z = 6$), where the system size of each layer is taken as: $N_x = 3$ and $N_y = 3$. The red and the blue curves correspond to the results for the smoothly varying and the conventional disordered films, respectively.

function, and accordingly, we determine the typical current amplitude (I_{typ}) by averaging over a large number (50) of random disordered configurations in each case to achieve much more accurate result. On the other hand, for the averaging over the bias voltage (V), we compute the results considering the range of V within -16 to 16 in each case. In this present study, we concentrate ourselves only on the smaller system sizes, since all the qualitative behaviors remain invariant even for the larger system sizes, and therefore, the numerical results can be computed in the low cost of time. The variation of the typical current amplitudes (I_{typ}) as a function of the impurity strength (W) for the thin films

with system size $N_x = 3$, $N_y = 3$ and $N_z = 6$ is shown in Fig. 2. The red and the blue curves correspond to the results for the smoothly varying and the conventional disordered films, respectively. For the conventional disordered film, the typical current amplitude decreases sharply with the increase of the impurity strength (W). This behavior can be well understood from the theory of Anderson lo-

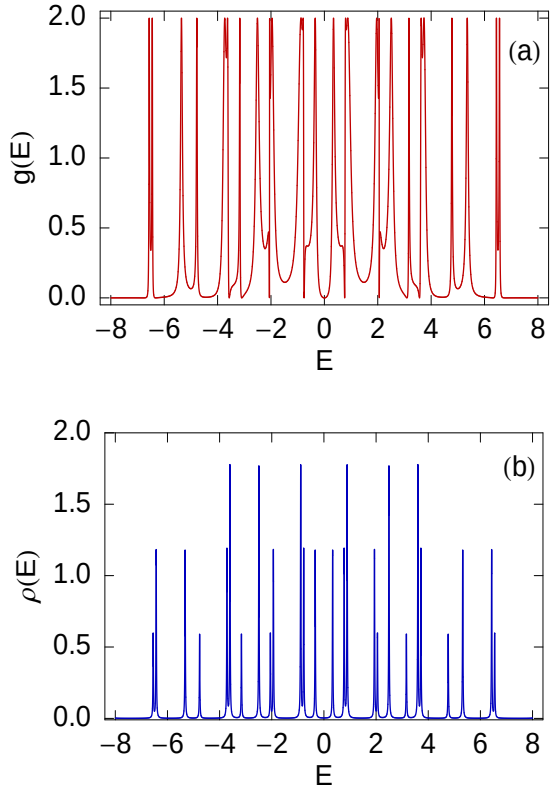

Figure 3: (a) $g(E)$-E (red color) and (b) $\rho(E)$-E (blue color) curves for an ordered ($W = 0$) thin film with six layers ($N_z = 6$), where the system size of each layer is taken as: $N_x = 3$ and $N_y = 3$.

calization, where more localization is achieved with the increase of the disorder strength [34]. Such a localization phenomenon is well established in the transport community from a long back ago. A dramatic feature is observed only when the disorder strength decreases smoothly from the top most highest disordered layer, keeping the lowest bottom layer as disorder free. In this particular system, the current amplitude initially decreases with the increase of the impurity strength, while beyond some critical value of the impurity strength $W = W_c$ (say) the amplitude increases. This phenomenon is completely opposite in nature from the traditional disordered system, as discussed above. Such an anomalous behavior can be explained in this way. We can treat the smoothly varying disordered film with ordered bottom layer as an order-disorder separated film. In such an order-disorder separated film, a gradual separation of the energy spectra of

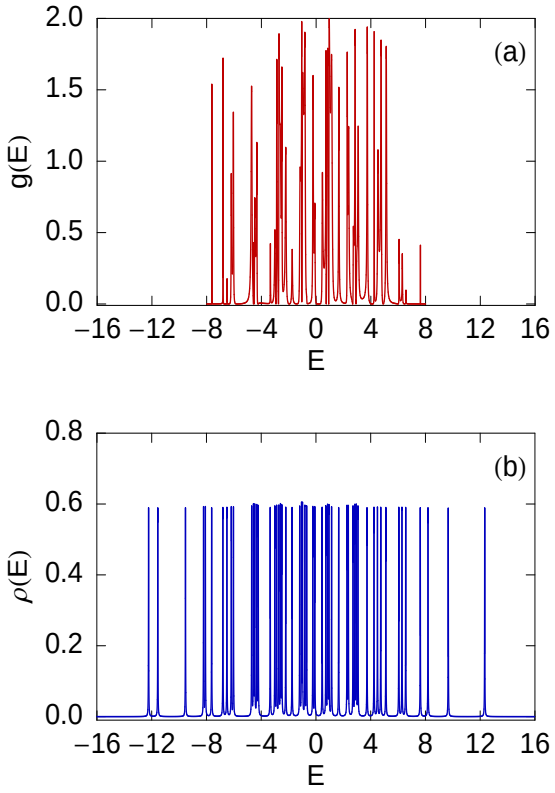

Figure 4: (a) $g(E)$-E (red color) and (b) $\rho(E)$-E (blue color) curves for a smoothly varying disordered ($W = 10$, weak disorder limit) thin film with six layers ($N_z = 6$), where the system size of each layer is taken as: $N_x = 3$ and $N_y = 3$.

the disordered layers and the ordered layer takes place with the increase of the disorder strength W. In the limit of strong disorder, the energy spectrum of the order-disorder separated film contains localized tail states with much small and central states with much large values of localization length. Hence the central states gradually separated from the tail states and delocalized with the increase of the strength of the disorder. To understand it precisely, here we present the behavior of the conductance for the three different cases considering the disorder strengths $W = 0$, $W = 10$ and $W = 30$. The results are shown in Fig. 3, Fig. 4 and Fig. 5, respectively. In every case the pictures of the den-

sity of states (DOS) are also given to show clearly that with the increase of the disorder strength more energy eigenstates appear in the energy regimes for which the conductance is zero. Thus the separation of the localized and the delocalized eigenstates is clearly visible from these pictures. Hence for the coupled order-disorder separated film, the coupling between the localized states with the extended states is strongly influenced by the strength of the

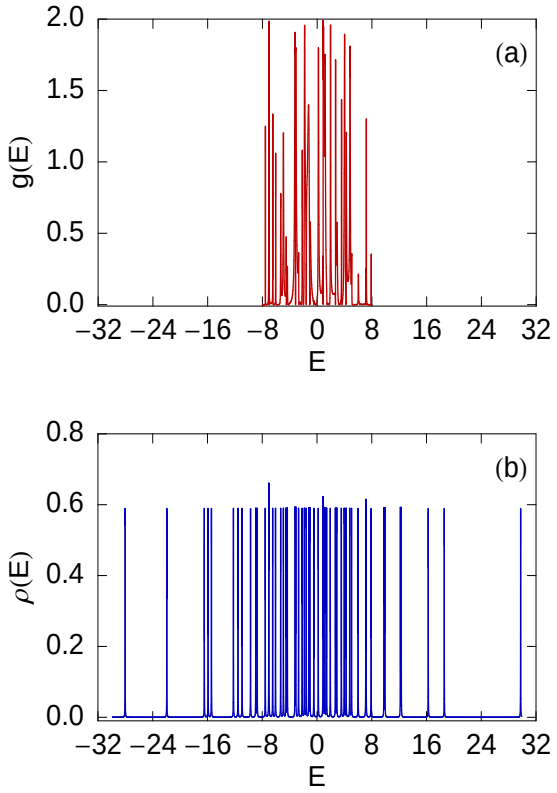

Figure 5: (a) $g(E)$-E (red color) and (b) $\rho(E)$-E (blue color) curves for a smoothly varying disordered ($W = 30$, strong disorder limit) thin film with six layers ($N_z = 6$), where the system size of each layer is taken as: $N_x = 3$ and $N_y = 3$.

disorder, and this coupling is inversely proportional to the disorder strength W which indicates that the influence of the random scattering in the ordered layer due to the strong localization in the disordered layers decreases. Therefore, in the limit of weak disorder the coupling effect is strong, while the coupling effect becomes less significant in the strong disorder regime. Accordingly, in the limit of weak disorder the electron transport is strongly influenced by the impurities at the disordered layers such that the electron states are scattered more and hence the current amplitude decreases. On the other hand, for the strong disorder limit the extended states are less influenced by the disordered layers and the coupling effect gradually decreases with the increase of the impurity strength which provide the larger current amplitude in the strong disorder limit. For large enough impurity strength, the extended states are almost unaffected by the impurities at the disordered layers and in that case the current is carried only by these extended states in the ordered layer which is the trivial limit. So the exciting limit is the intermediate limit of W. In order to investigate the finite size effect on the electron transport, we also calculate the typical current amplitude for the other two different system sizes of the thin film those are plotted in Fig. 6 and Fig. 7, respectively. In Fig. 6, we plot the typical

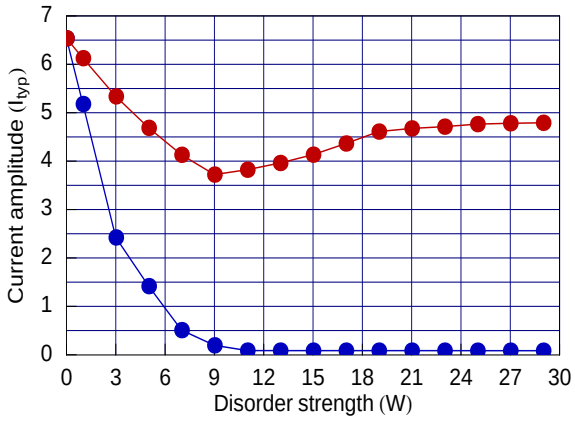

Figure 6: Typical current amplitudes (I_{typ}) as a function of the impurity strength (W) for the thin films with seven layers ($N_z = 7$), where the system size of each layer is taken as: $N_x = 3$ and $N_y = 3$. The red and the blue curves correspond to the identical meaning as in Fig. 2.

current amplitudes for the films with system size $N_X = 3$, $N_y = 3$ and $N_z = 7$, while the results for the films with system size $N_x = 3$, $N_y = 3$ and $N_z = 8$ are shown in Fig. 7. The red and the blue curves of these two figures correspond to the identical meaning as in Fig. 2. Since both for these two films we will get the similar behavior of the conductance and the density of states, we do not describe these results further. The variation of the typical current amplitudes for these films with the disorder strength shows quite similar behavior as discussed earlier. But the significant point is that the typical current amplitude where it goes to a minimum strongly depends on the system size of the film which reveals the finite quantum size effects in

the study of electron transport phenomena. The underlying physics behind the location of the minimum in the current versus disorder curve is very interesting. The current amplitude is controlled by the two competing mechanisms. One is the random scattering in the ordered layer due to the localization in the disordered layers which tends to decrease the current, and the other one is the vanishing influence of random scattering in the ordered layer due to the strong localization in the disordered layers which provides the enhancement of the current. Now depending on the ratio of the atomic sites in the disordered region to the atomic sites in the ordered region, the vanishing effect of random scattering from the ordered states dominates over the non-vanishing effect of random scattering from these states for a particular disorder strength ($W = W_c$), which provides the location of the minimum in the current versus disorder curve.

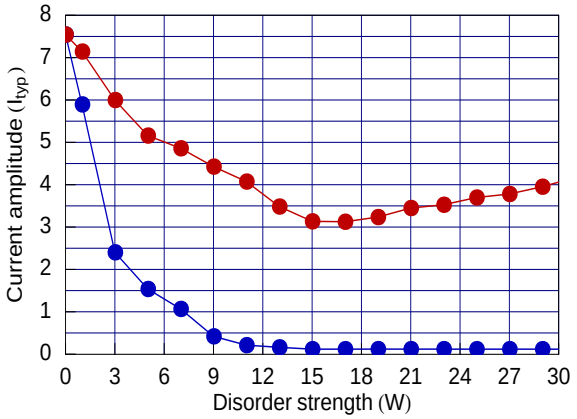

Figure 7: Typical current amplitudes (I_{typ}) as a function of the impurity strength (W) for the thin films with eight layers ($N_z = 8$), where the system size of each layer is taken as: $N_x = 3$ and $N_y = 3$. The red and the blue curves correspond to the identical meaning as in Fig. 2.

4 Concluding Remarks

In conclusion, we have investigated a novel feature of disorder on electron transport through a thin film of variable disorder strength from its surface attached to two metallic electrodes by the Green's function formalism. A simple tight-binding model has been used to describe the film, where the coupling to the electrodes has been treated through the use of Newns-Anderson chemisorption theory. Our results have predicted that, in the smoothly varying disordered film the typical current amplitude increases with the increase of the disorder strength in the strong disorder regime, while the amplitude decreases in the weak disorder regime. This behavior is completely opposite to that of the conventional disordered film, where the current amplitude always decreases with the disorder strength and such a strange phenomenon has not been pointed out previously in the literature. In this context we have also discussed the finite size effect on the electron transport by calculating the typical current amplitude in different film sizes. From these results it has been observed that, the typical current amplitude where it goes to a minimum strongly depends on the size of the film which manifests the finite size effect on the electron transport. Thus we can predict that, there exists a strong correlation between the localized states at the disordered layers and the extended states in the ordered layer which depends on the strength of the disorder, and it provides a novel phenomenon in the transport community. Similar type of anomalous quantum transport can also be observed in lower dimensional systems like, edge disordered graphene sheets of single-atom-thick, surface disordered finite width rings, nanowires, etc. Our study has suggested that the carrier transport in an order-disorder separated mesoscopic device may be tailored to desired properties through doping for different applications.

Throughout our discussions we have used several realistic approximations by neglecting the effects of the electron-electron interaction, all the inelastic scattering processes, the Schottky effect, the static Stark effect, etc. More studies are expected to take into account all these approximations for our further investigations.

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